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Cooperative Research Alliance

Multiscale Modeling of Electronic Materials (MSME)

Dr. Meredith L. Reed

ARL Opportunities Conference

November 19, 2010

Fairfax, VA

US ARMY RDECOM

ARL

US ARMY RDECOM

ARL Major Laboratory Programs

Protection
- Materials and Manufacturing Science for Protection
- Vehicle Protection
- Individual Warfighter Protection

Lethality
- Energetic Materials and Propulsion
- Projectiles, Warheads and Scalable Effects
- Materials and Manufacturing Science for Lethality
- Affordable Precision Munitions
- Advanced Weapons Concepts

Human Dimension
- Soldier Sensory-Cognitive Motor Performance
- Neuroergonomics
- Social-Cognitive-Cultural Networks
- Human Robotic Interaction
- Human Systems Integration

Survivability/Lethality Analysis
- Ballistic Vulnerability/Lethality
- Electronic Warfare
- Information Assurance and Computer Network Defense
- Systems of Systems

Networks
- Information Sciences
- Network Sciences
- Battlefield Environment
- Advanced Computing and Computational Sciences

Extramural Basic Research
- Chemistry
- Physics
- Life Sciences
- Network Science
- Environmental Sciences
- Materials Sciences
- Mechanical Sciences
- Mathematics
- Computing Science
- Electronics

Sensors
- RF Technologies
- Electronics Technologies
- EO/IR Technologies
- Non-Imaging Technologies
- Sensor Processing

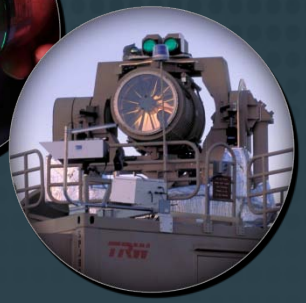
Power and Energy
- Power Generation and Conversion
- Energy Storage
- Power Control and Distribution
- Thermal Management
- Energy Science

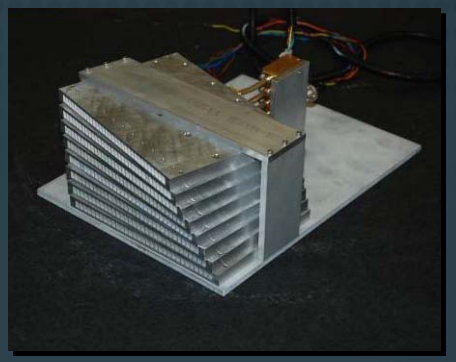
Mobility and Logistics
- Platform Mechanics
- Vehicle Propulsion
- Autonomous Systems
- Reliability

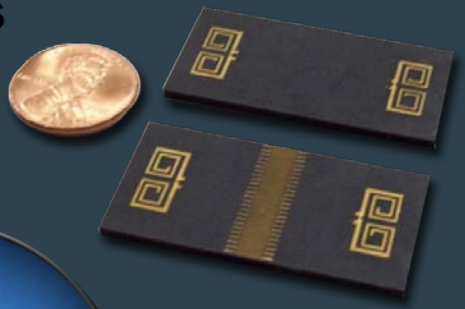
Simulation & Training
- Intelligent Technologies for Training
- Synthetic Environments
- Immersive Learning
- Training Application Environments
- Advanced Distributed Simulation

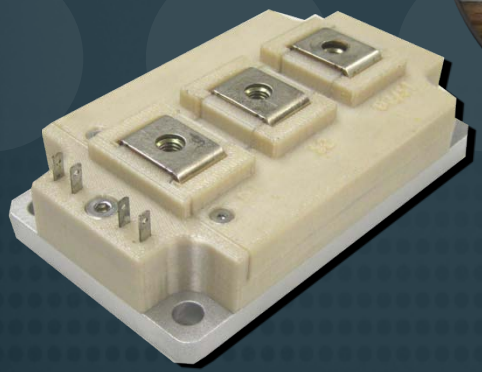
Sensors

- RF Technologies
- EO/IR Technologies
- Non-Imaging Technologies
- Electronics Technologies
- Sensor Processing









Power and Energy

- Power Generation & Conversion
- Power Control & Distribution
- Energy Storage
- Thermal Management

Sensors and Electron Devices

ELECTRO-OPTICS & PHOTONICS

- EO Materials & Devices
- Microphotonics
- Optics
- Optics & Photonics Technology Integration

ELECTRONICS & RF

- Micro & Nano Materials and Devices
- Electronics Technology
- Antennas & RF Technology Integration
- RF Signal Processing & Modeling

SIGNAL & IMAGE PROCESSING

- Acoustics & EM Sensing
- ISR Technology Integration
- Image Processing
- Networked Sensing & Fusion

ENERGY & POWER

- Electro-chemistry
- Power Components
- Power Conditioning

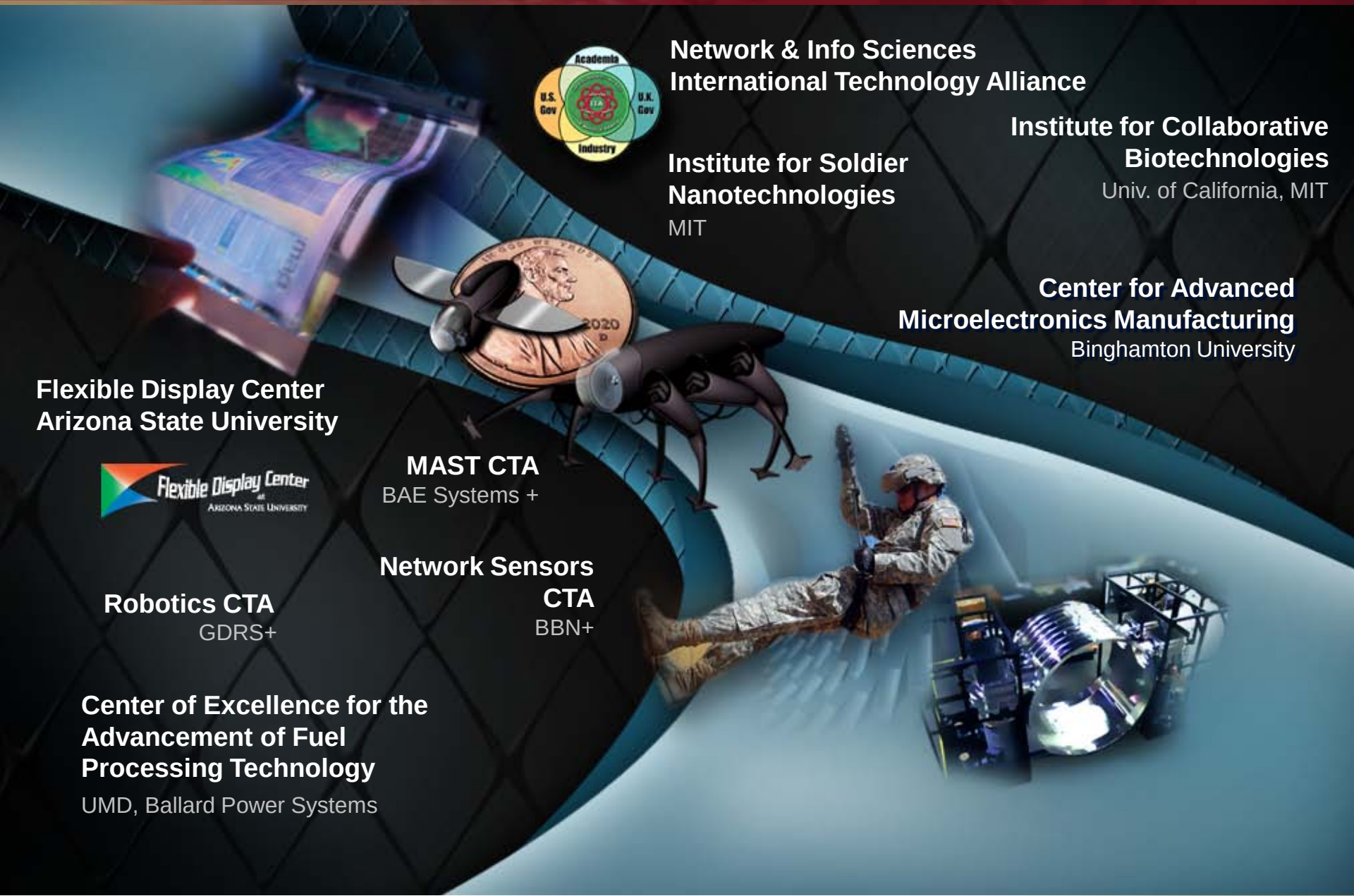
SPECIAL PROGRAMS OFFICE

SENSORS & ELECTRONICS INTEGRATION TECH OFFICE

US ARMY RDECOM

Collaborative Ventures

ARL



Network & Info Sciences International Technology Alliance

Institute for Soldier Nanotechnologies
MIT

Institute for Collaborative Biotechnologies
Univ. of California, MIT

Center for Advanced Microelectronics Manufacturing
Binghamton University

Flexible Display Center Arizona State University

Flexible Display Center at Arizona State University

MAST CTA
BAE Systems +

Network Sensors CTA
BBN+

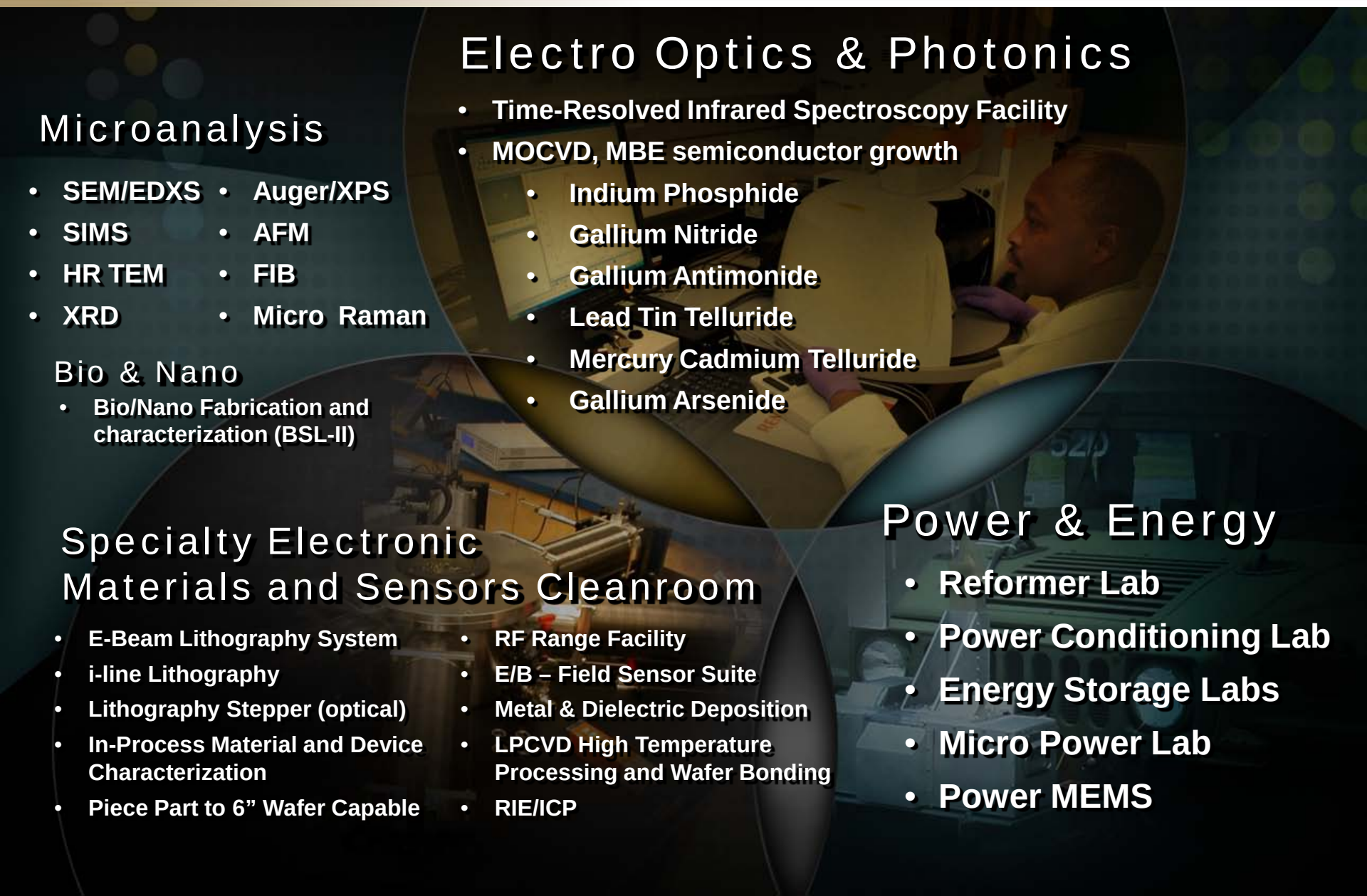
Robotics CTA
GDRS+

Center of Excellence for the Advancement of Fuel Processing Technology
UMD, Ballard Power Systems

US ARMY RDECOM

Infrastructure & Capabilities

ARL



Electro Optics & Photonics

- Time-Resolved Infrared Spectroscopy Facility
- MOCVD, MBE semiconductor growth
  - Indium Phosphide
  - Gallium Nitride
  - Gallium Antimonide
  - Lead Tin Telluride
  - Mercury Cadmium Telluride
  - Gallium Arsenide

Microanalysis

- SEM/EDXS
- SIMS
- HR TEM
- XRD
- Auger/XPS
- AFM
- FIB
- Micro Raman

Bio & Nano

- Bio/Nano Fabrication and characterization (BSL-II)

Specialty Electronic Materials and Sensors Cleanroom

- E-Beam Lithography System
- i-line Lithography
- Lithography Stepper (optical)
- In-Process Material and Device Characterization
- Piece Part to 6” Wafer Capable
- RF Range Facility
- E/B – Field Sensor Suite
- Metal & Dielectric Deposition
- LPCVD High Temperature Processing and Wafer Bonding
- RIE/ICP

Power & Energy

- Reformer Lab
- Power Conditioning Lab
- Energy Storage Labs
- Micro Power Lab
- Power MEMS

Sensors: Infrastructure & Capabilities

US ARMY RDECOM

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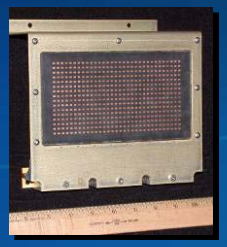
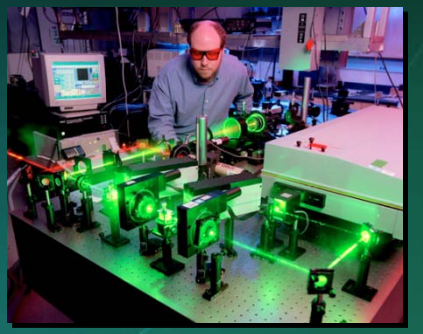


Radar, Antenna & MFRF

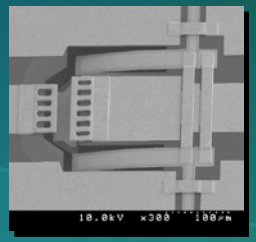
Spectral dissection of bacteria and thin-films



Non-linear Optics

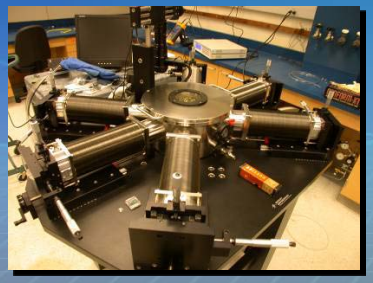
RF Material & Devices

Electric Field Cage for sensor evaluation



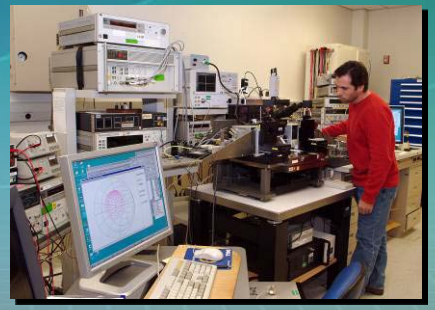
NEMS & MEMS PZT

Device Fabrication Advanced RF Technology



DC-40GHz environmental cryogenic I/V probe station

Piezoelectric Sputtering for MEMS and communication devices



Electronic transport characterization in nano-scale structures

III-V Etching for optical device fabrication

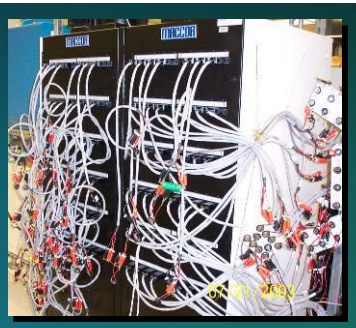
Device Fabrication Electro-Optics

Power & Energy: Infrastructure & Capabilities

Jet Vapor Deposition

Dry Room for electrochemical cell preparation

Single and multiple battery cell evaluation laboratories

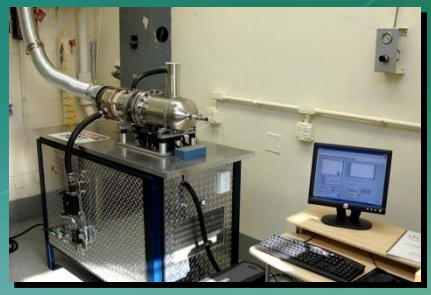


Isomer Battery Laboratory

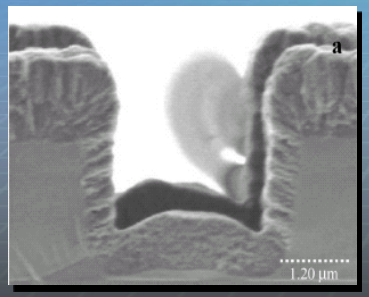
Electric Drive

Power Conditioning Lab

Fuel Cell evaluations

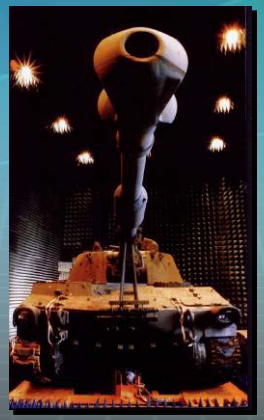


Small Engine Evaluation



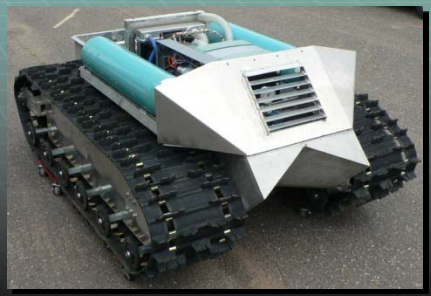
SiC device stress analysis evaluations

Air Gun for high-G evaluation



High Power RF Anechoic Chamber

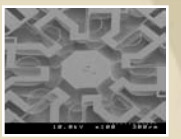
Fuel Cell Powered Robotic Vehicle

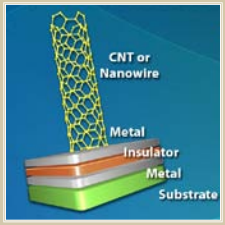


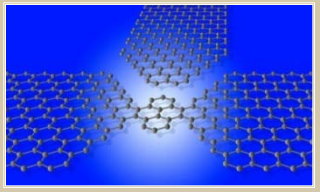
Sensing and Energy and Power Research Continuum

Area Surveillance and Tracking

MEMS Sensors and actuators for microrobots



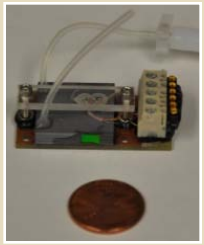




Graphene

Family of UGS

Compact Radar



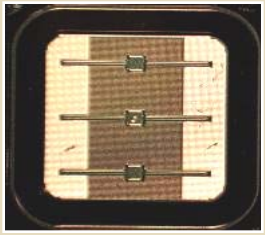
Environmental Sensing

Energy Harvesting Rectenna

Flexible Electronics

Reformed Methanol Fuel Cell

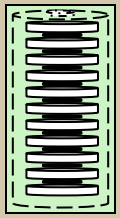
Traction Module Power Conversion Switches



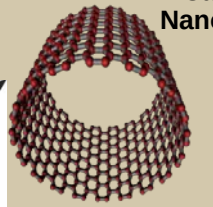
Wide Bandgap Devices

Li-Air Prototype Cells

Isotope Energy Source in a AA-battery Package

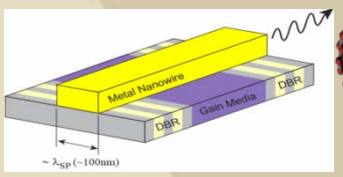


Carbon Nanotubes

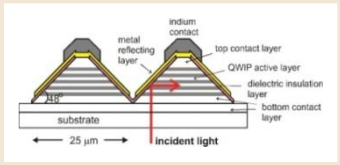


Flexible Displays

High Voltage Li-Ion Electrolytes



Photonics & Electronics Integration

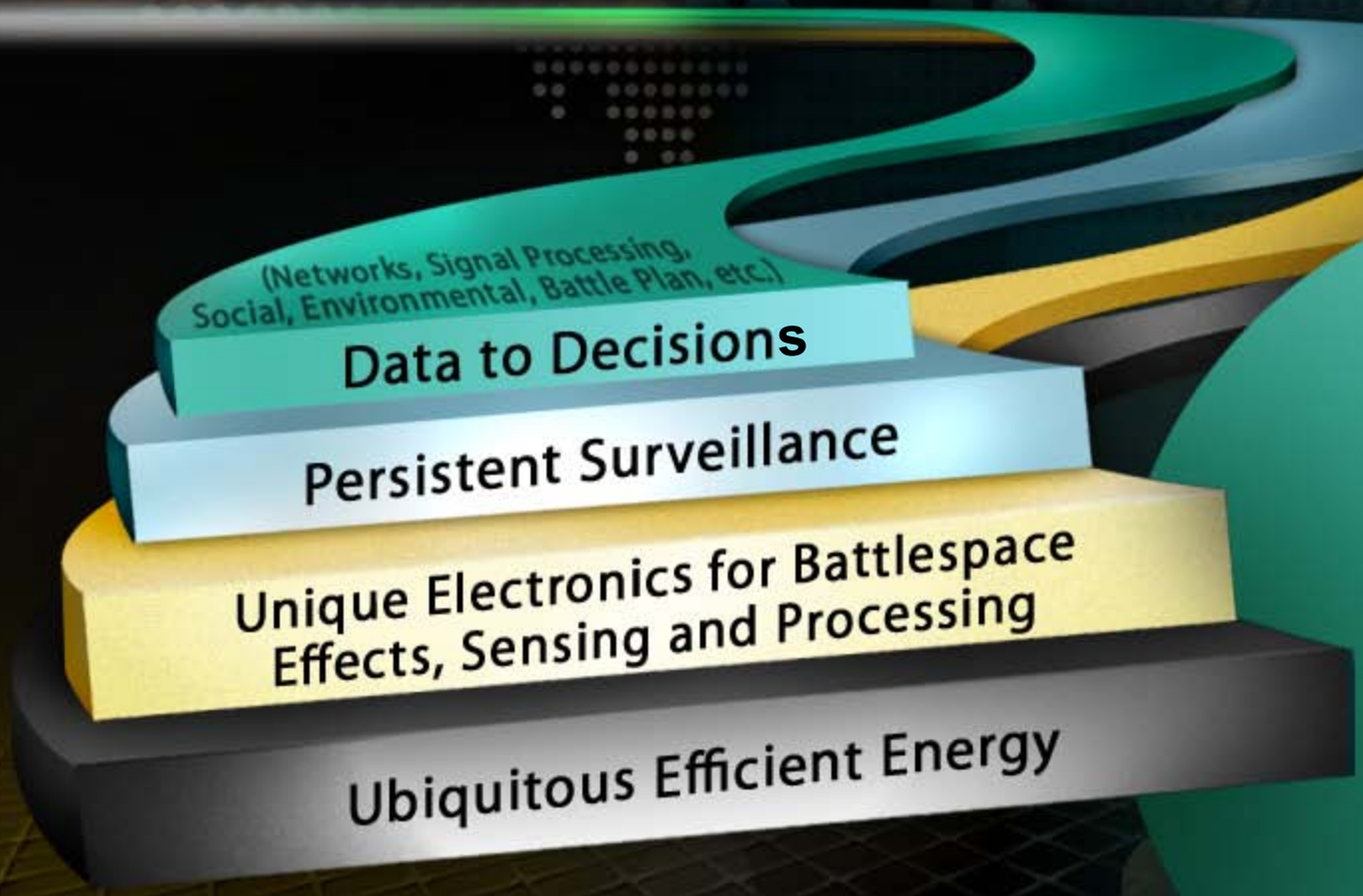


C-QWIP FPAs

Accomplishments — Near Term — Future

Disruptive Sensors and Electronics for C4ISR Superiority and Advanced Energy and Power for Warfighter Dominance

STRATEGIC DIRECTION

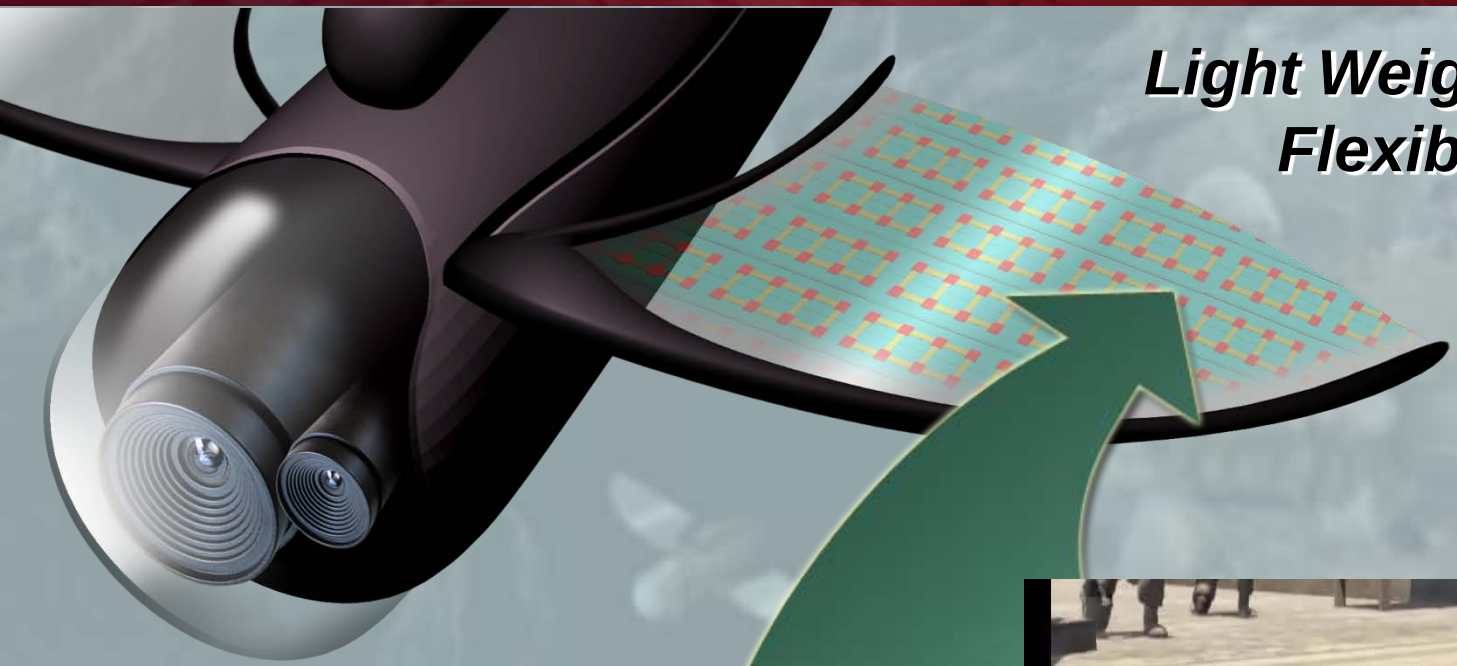


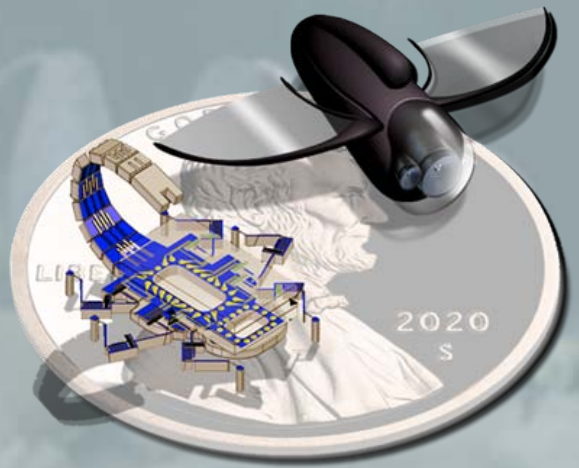
Warfighter Outcomes

- Counter IED & Mine
- Mission Command
- Training
- Power & Energy
- Human Dimension
- Force Protection
- Battlespace Awareness
- Force Application
- Logistics
- Unmanned Systems Operations


MODEL ECL-1054A
SMALL RADAR

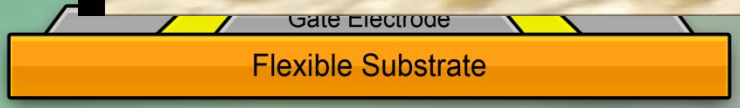
Light Weight, Flexible Electronics





CMOS, Pr
Logic, D

Sou



Technical Synergies

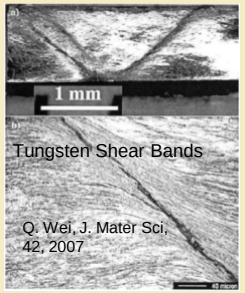
Multi-Scale Mat. Behavior in Ultra High Loading Rate Environments

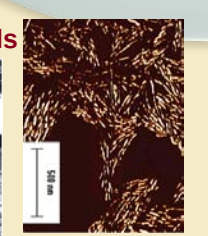
- Investigate bridging scales
- Develop models & simulations
- Develop innovative experimentation & validation techniques
- Define multiscale material metrics
- Perform processing & synthesis

Electronic Materials

- Explore material designs for electrochemical energy,
- Develop hybrid photonic, spintronic devices
- Investigate and develop heterogeneous metamorphic electronics

Protection Materials





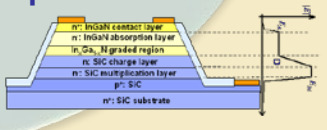
Designer Microstructure Composites

Army-relevance

Underpinning science infusion

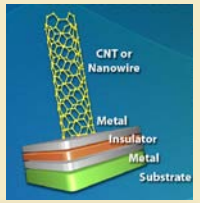
Army-relevance

Electronics



Opto-electronics

Power & Energy



In-house Cross-Disciplinary Multiscale Research of Materials Initiative

- **Underpinning Multiscale Physics & Chemistry Fundamentals**
- **Computational Science Environments, Codes & Software Tools**
- **Validation & Verification**

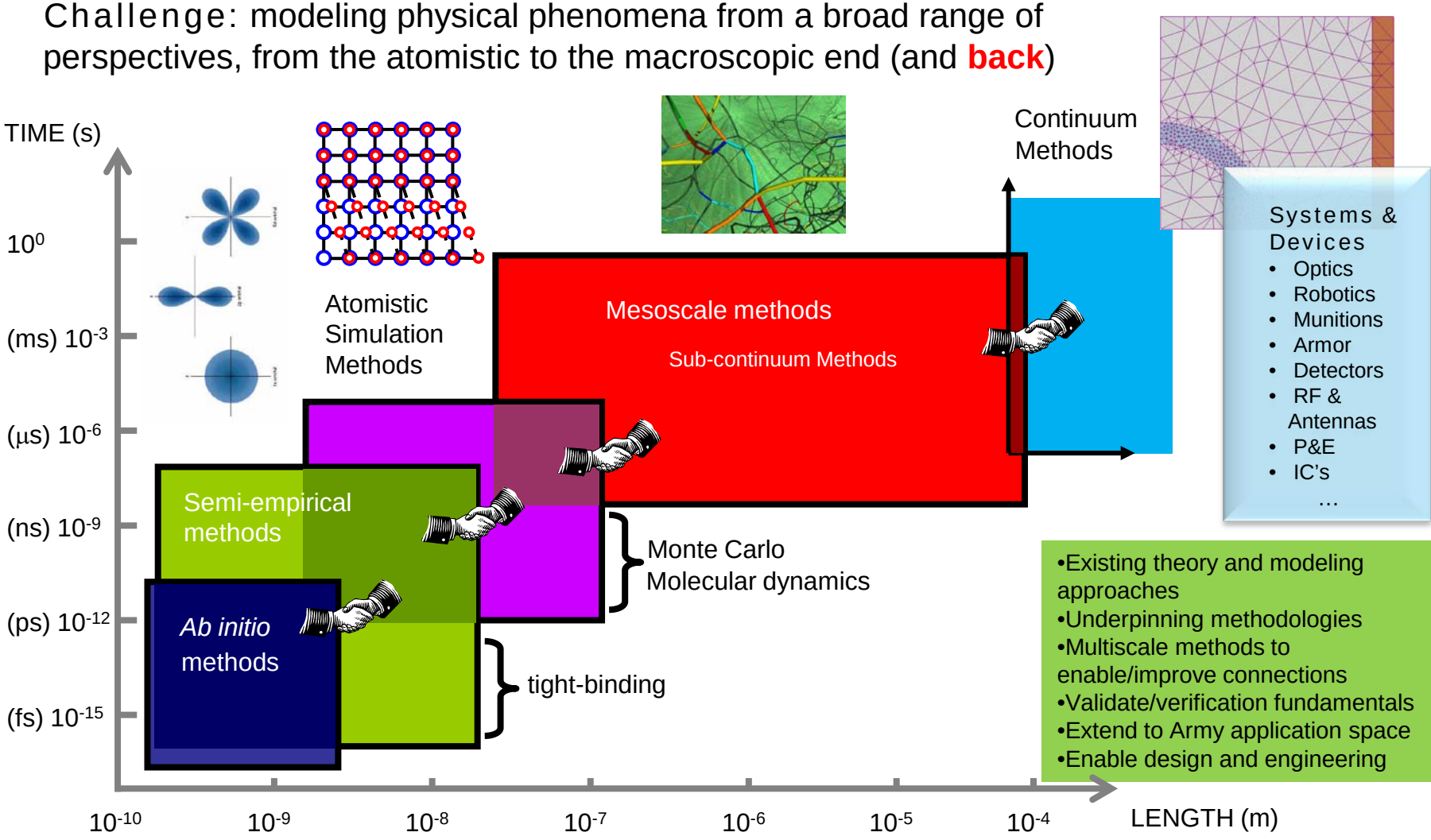
Motivation

Multiscale Modeling of Electronic Materials

- To enable the quantitative understanding of electronic materials from the smallest to the largest relevant scales
- Resulting models are needed to create new understanding and improved electronic device applications to include sensors and electronics for enhanced battlespace effects, and efficient power and energy devices

Multiscale Modeling of Materials

Challenge: modeling physical phenomena from a broad range of perspectives, from the atomistic to the macroscopic end (and **back**)



Large jumps are easier than smaller intimate jumps.

ARL Multi-Scale Multi-Disciplinary Modeling of Electronic Materials Workshop

Aug 31 – Sep 1 2010

Fairfax, Virginia 22033

Opportunities for Multiscale Modeling of Electronic Materials

Electrochemistry	**Focus on interfacial physics and chemistry; nano structures, solid-liquid interface–clear opportunities for batteries, capacitors, fuel cells, etc.**
Photonic Interactions	**Interaction of photons, electrons, phonons–in other words, photonics, spintronics, plasmonics, and phonons**
Heterogeneous Metamorphic Electronics	**Mixed materials, with partial ordering–includes graphene, metamaterials, nanoelectronic structures, etc.**

Objectives

- Execute a focused basic research program to realize a materials by design capability
- Drive forward and expand the fundamental understanding in the area of multi-scale/multidisciplinary materials behavior to directly improve the performance of electronic materials.
- Create a framework that enhances and fosters cross disciplinary and cross organizational collaboration that brings a team of academia, industry and government together to address critical focused research in Multiscale Modeling of Electronic Materials

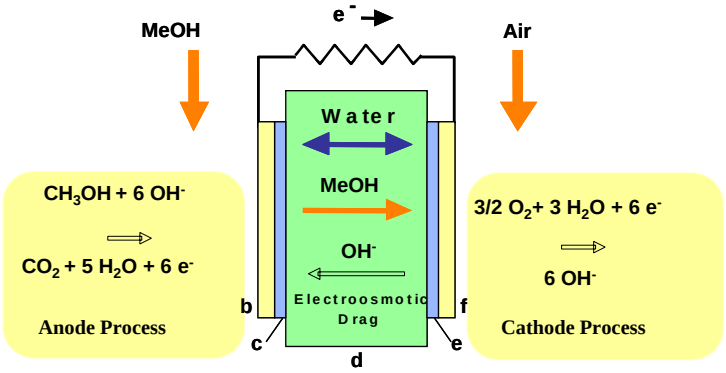
Electronic Materials Research Areas for MSME CRA

Electrochemistry	**Focus on interfacial physics and chemistry; nano structures, solid-liquid interface–clear opportunities for batteries, capacitors, fuel cells, etc.**
Photonic Interactions	**Interaction of photons, electrons, phonons–in other words, photonics, spintronics, plasmonics, and phonons**
Heterogeneous Metamorphic Electronics	**Mixed materials, with partial ordering–includes graphene, metamaterials, nanoelectronic structures, etc.** **– Interfaces of dissimilar materials** **– Defects**

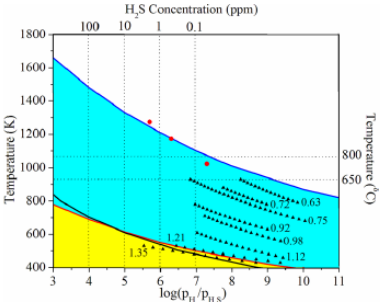
Note: Asking for CRA proposals to include a plan for incorporating "Hybrid Organic Electronics" in future years

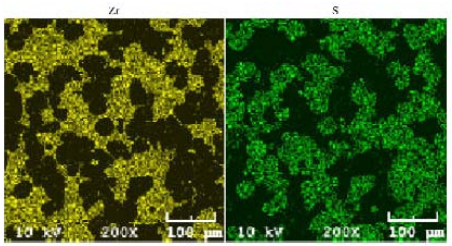
Electrochemical Energy Devices : Existing SEDD Materials Research Programs (examples)

Alkaline Membrane Fuel Cells

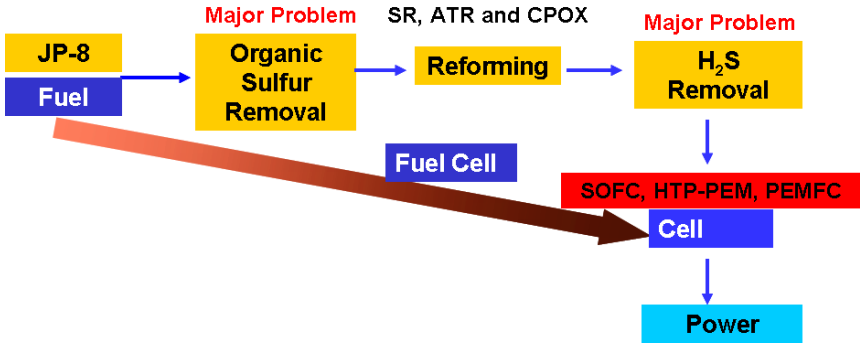


Long-Term Interest – Solid Oxide Fuel Cells



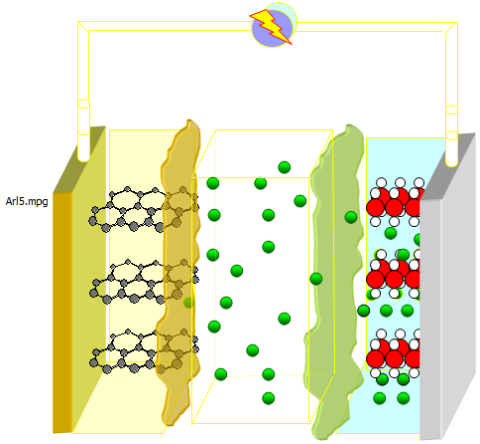


Logistics Fuel Processing

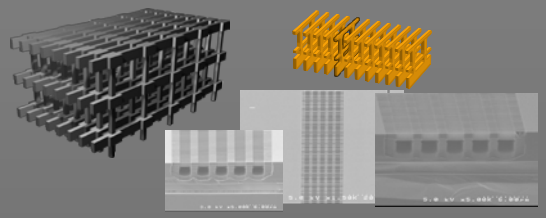


Li-ion Batteries

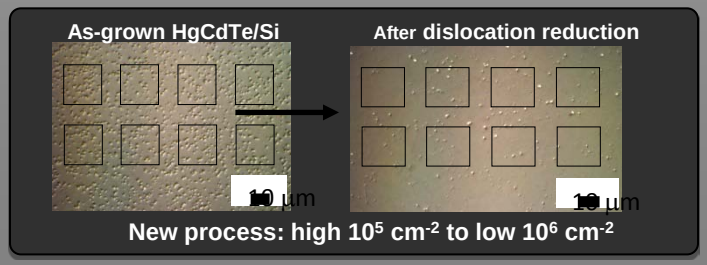
- **Energy density: 200 Wh/kg; Power density: 4 kW/kg at 60 Wh/kg**
- **Insertion types of cathode and anode for high rechargeablity**
- **Protective solid electrolyte interphase (SEI) for long cycle and storage life**



Hybrid Photonic, Spintronic Devices : Existing SEDD Materials Research Programs (examples)

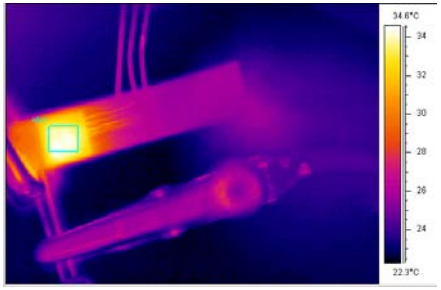


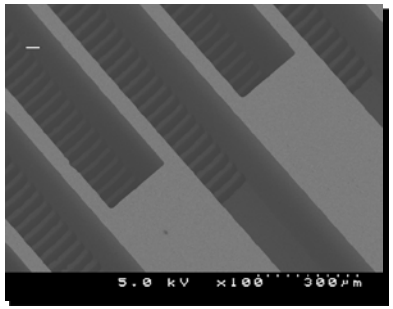
III-Nitrides

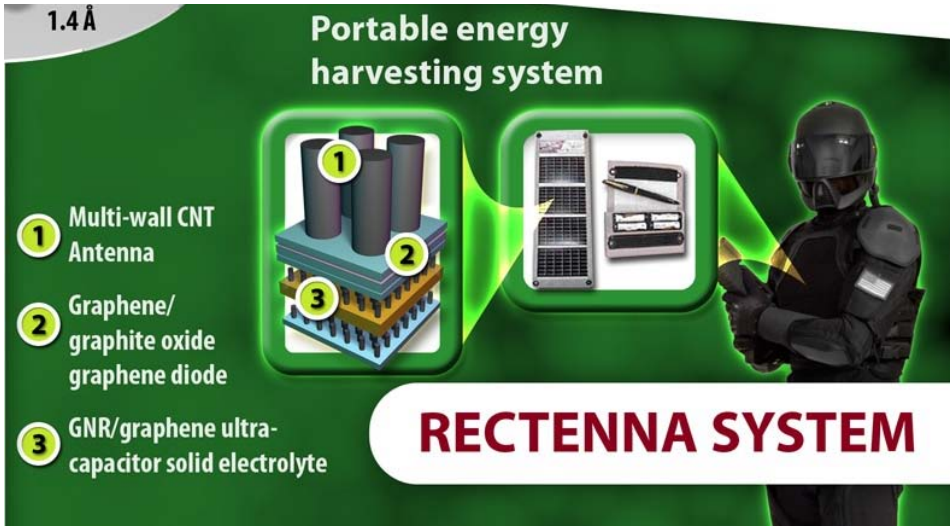


Heterogeneous Metamorphic Electronics: Existing SEDD Materials Research Programs (examples)

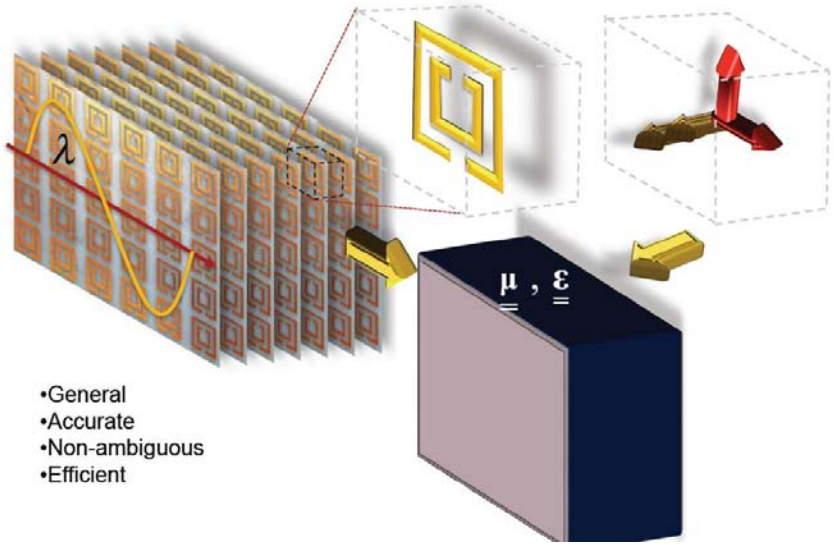
WBG Semiconductor Power Devices



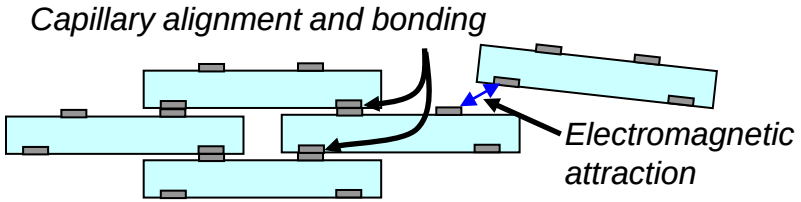




Meta-materials for RF/Antennas



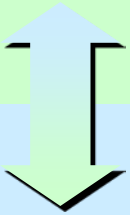
Heterogeneous Integration via Fluidic self-assembly



Multiscale Modeling Research Areas:

Performed for each of the Electronic Materials Research Areas

External CRA Effort



ARL CRA Effort

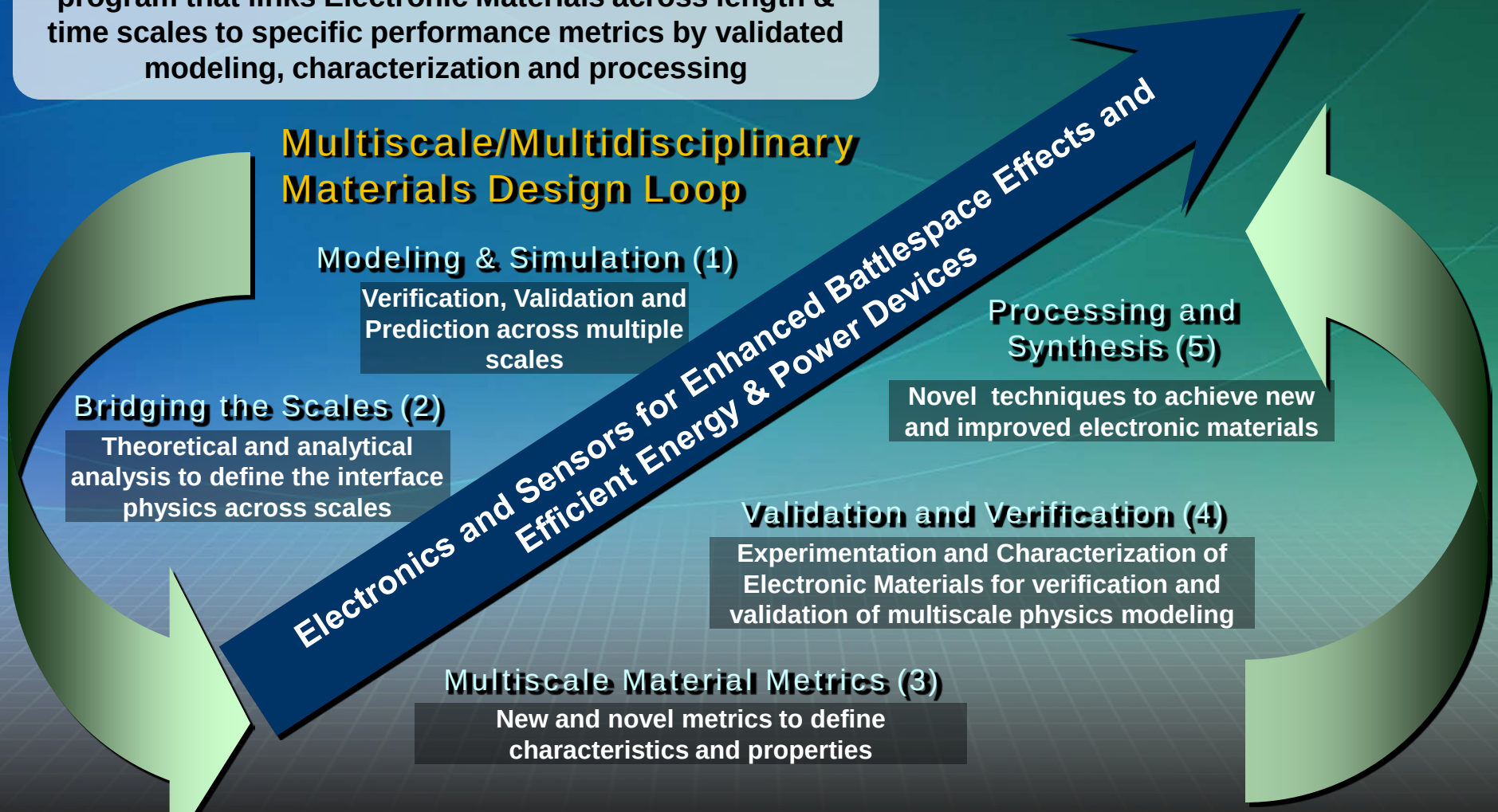
- **Modeling and Simulation:** Validated multiscale modeling of electronic materials design materials and predict performance by exploiting the hierarchy of scales in a multidisciplinary environment
- **Bridging the Scales: Analysis, Theory and Algorithms:** Validated theoretical and analytical analyses to effectively define the interface physics across length scales and disciplines
- **Multiscale Modeling Material Metrics:** A comprehensive set of metrics that electronic material for each of the three Electronic Materials Research Areas defined above to enable the enhancement or creation of new electronic devices
- **Validation and Verification:** Comprehensive validated experimental capabilities bridging time and space for probing the physics and mechanisms of electronic materials and for verification and validation of multiscale/multidisciplinary physics modeling.
- **Processing and Synthesis:** Validated modeling and techniques for the synthesis and processing of Electronic Materials.

MSME CRA Program Strategy

Approach

Cohesive, multidisciplinary collaborative research program that links Electronic Materials across length & time scales to specific performance metrics by validated modeling, characterization and processing

Electronic Materials for U.S. Army Systems



MSME CRA Program Announcement (PA)

- Formulate a program to demonstrate the ability to achieve the research and programmatic goals of the CRA as outlined in the PA
- Define and outline the strategy for executing the materials by design loop and identify how the program will achieve the specific research goals in the five Multiscale Modeling Research Areas and how they will be integrated and interfaced within the materials by design loop
- Identify how the program will address the five Multiscale Modeling in each of the three Electronic Materials Research Areas: (1) Electrochemical Energy Devices; (2) Hybrid Photonic, Spintronic Devices; and (3) Heterogeneous Metamorphic Electronics
- Define the metrics by which success is expected to be measured
- Identify the strategy, plans and methods for collaboration essential to the success of the CRA
- Identify the optimal scientific, technical, programmatic and administrative team (expected to be comprised by a number of members) with the expertise to achieve the stated research goals and to oversee and manage finances, reporting, data, meetings, reviews and intellectual property

MSME CRA Collaboration

Collaboration to Achieve the CRA Research Goals

- **ARL Enterprise for Multiscale Research of Materials**
- **ARL SEDD Mission Program Internal to the CRA**

Education

- **Opportunities for Government Personnel**
- **Student Engagement with ARL Research Environment**

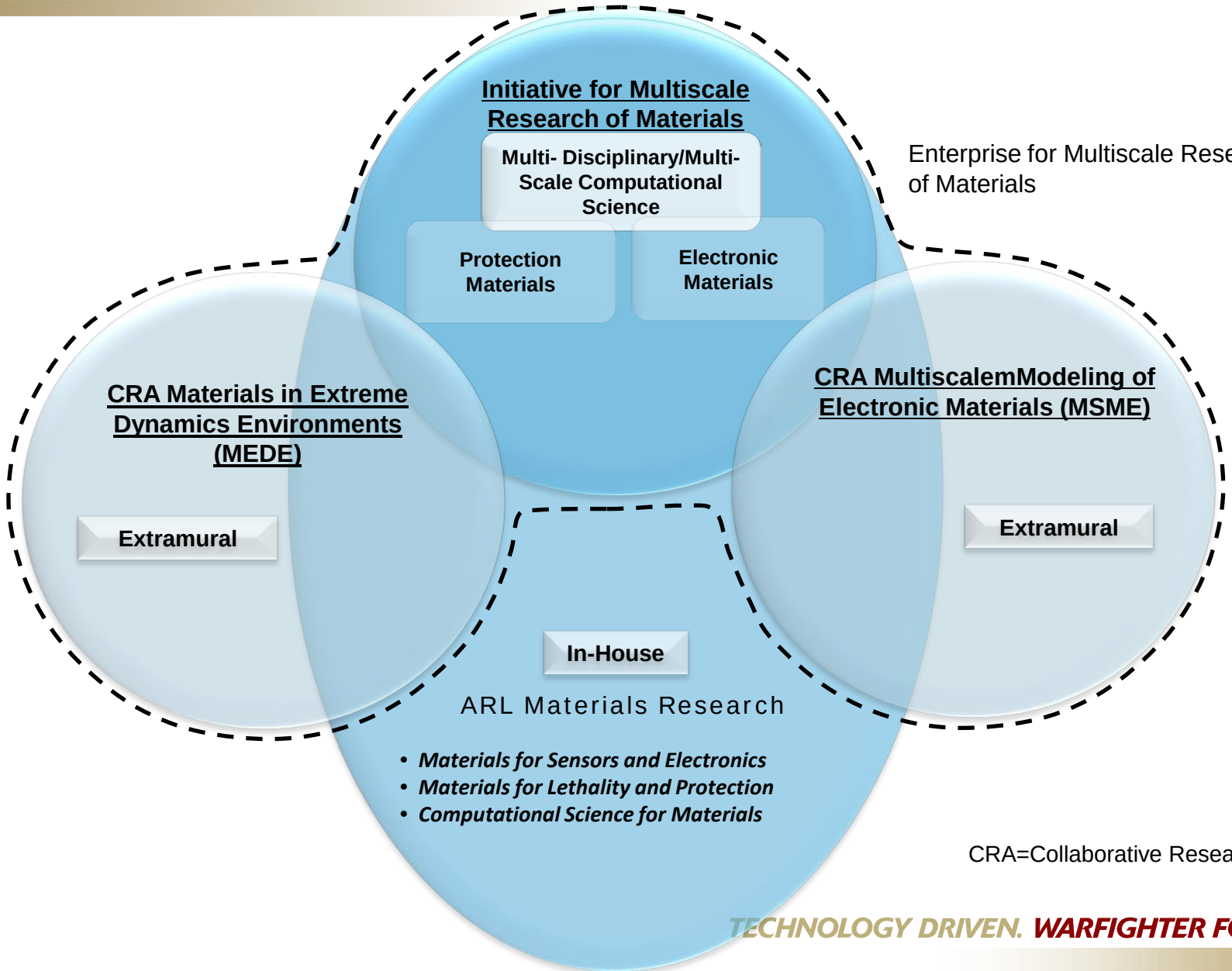
Other Collaboration Opportunities

- **High Performance Computing DoD Supercomputing Resource Center (HPC-DSRC)**
- **HPC (High Performance Computing) Software and Application Institute (HSAI) for Multi-Scale Reactive Modeling and Simulation of Insensitive Munitions (MSRMS-IM)**
- **Other Government Agencies (OGA's)**

Lectures, Workshops, and Research Reviews

Staff Rotation

MSME CRA Collaboration



Enterprise for Multiscale Research of Materials

CRA=Collaborative Research Alliance

MSME CRA Funding

CRA Basic Research Program

- **Basic Program funded for 5 Years with a 5 Year Option**
- **Start Second Quarter FY12**
- **Budget includes research costs, costs to manage the program, costs to collaborate and enable research transition**
- **Funding outlined in the PA are for planning purposes only**
- **Final funding is subject to Program Objective Memorandum Approval**

CRA Enhanced Basic and Applied Research Program

- **As the CRA proceeds it is anticipated that other Government agencies will be able to provide funding for specific research of interest**
- **This is currently unfunded**

Total Funded 5 Year Core Program $12.4M /Total Funded 10 Year Core Program $20.9M

SEDD MSME Open House

Thursday December 9th 2010

8:30 - 9:00 Arrival

9:00 - 12:00 SEDD Research Program and Tours

Army Research Laboratory-Adelphi Laboratory Center
2800 Powder Mill Rd
Adelphi, MD 20783

MSME CRA GOALS

Create a framework that enhances and fosters cross disciplinary and cross organizational collaboration that brings a team of academia, industry and government together to address critical focused research in Multiscale Modeling of Electronic Materials

2 Year Goals

- **Advance the fundamental understanding and implementation of Physics-Based Modeling of Electronic Materials across both time and space to develop set of algorithms/theories for a broad range of electronic materials to create new and/or improved electronic devices, and advance the understanding of existing performance**
- **Introduce interfaces, defects, imperfections**

5 Year Goals

- **Integrate new multidisciplinary /multi-scale physics to enable multi-scale modeling and simulation capability that is validated experimentally in time and space to apriori design new or improved electronic materials that are uniquely characterized, synthesized and processed.**
- Potential examples **of enhanced SoA resulting from the advancement or development of new theories and algorithms of MSME could include:**
  - **Higher performing (longer-lived) batteries by ~ 30% with more than double to treble the energy density**
  - **Increase efficiency by 20%, with a five fold increase in lifetime for UV solid state sources**

10 Year Goals

- **Advance the state of the art in multiscale modeling and electronic materials to create a capability for "Materials Optimization and Materials by Design"**
- **Deploy Multiscale Models for a variety of electronic materials that can be shared within the scientific community**